



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:59 am BST

PDB ID : 3BLS  
Title : AMPC BETA-LACTAMASE FROM ESCHERICHIA COLI  
Authors : Usher, K.C.; Shoichet, B.K.; Remington, S.J.  
Deposited on : 1998-06-04  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

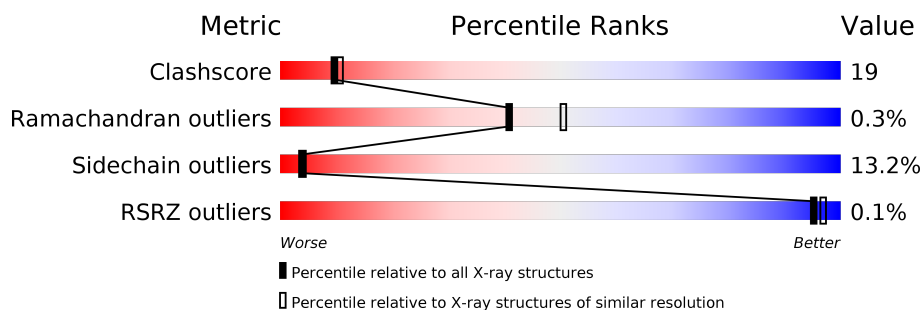
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	
1	B	358	

## 2 Entry composition [i](#)

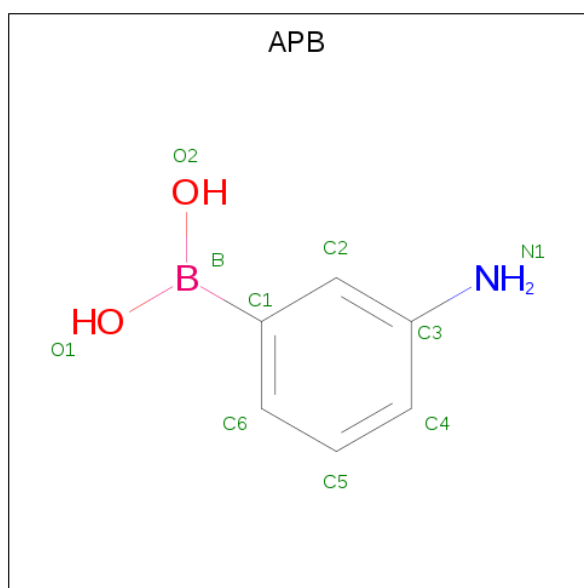
There are 3 unique types of molecules in this entry. The entry contains 5707 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AMPC BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	16	0	0
			2790	1799	474	511	6			
1	B	357	Total	C	N	O	S	13	0	0
			2790	1799	474	511	6			

- Molecule 2 is M-AMINOPHENYLBORONIC ACID (three-letter code: APB) (formula:  $C_6H_8BNO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			10	1	6	1	2		
2	B	1	Total	B	C	N	O	0	0
			10	1	6	1	2		

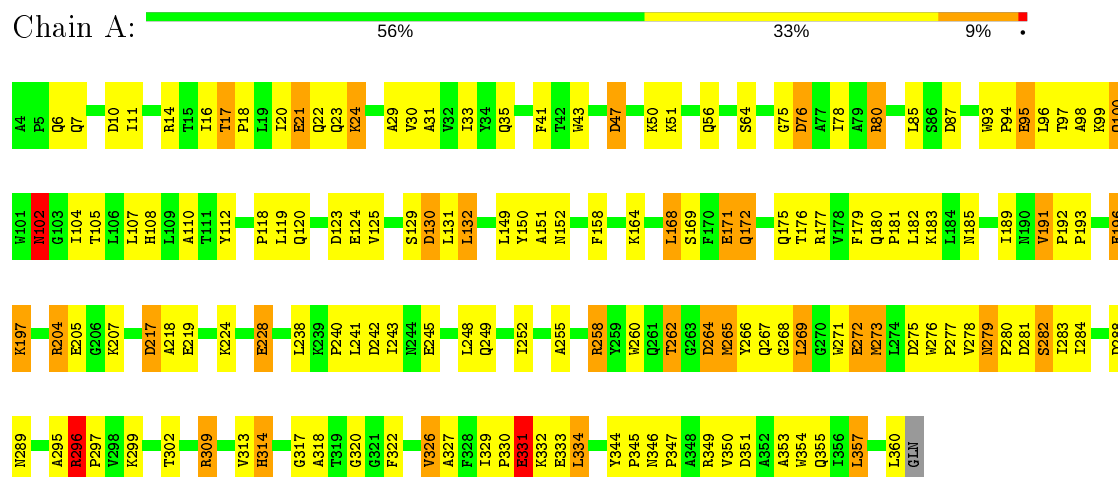
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	50	Total 50	O 50	0	0

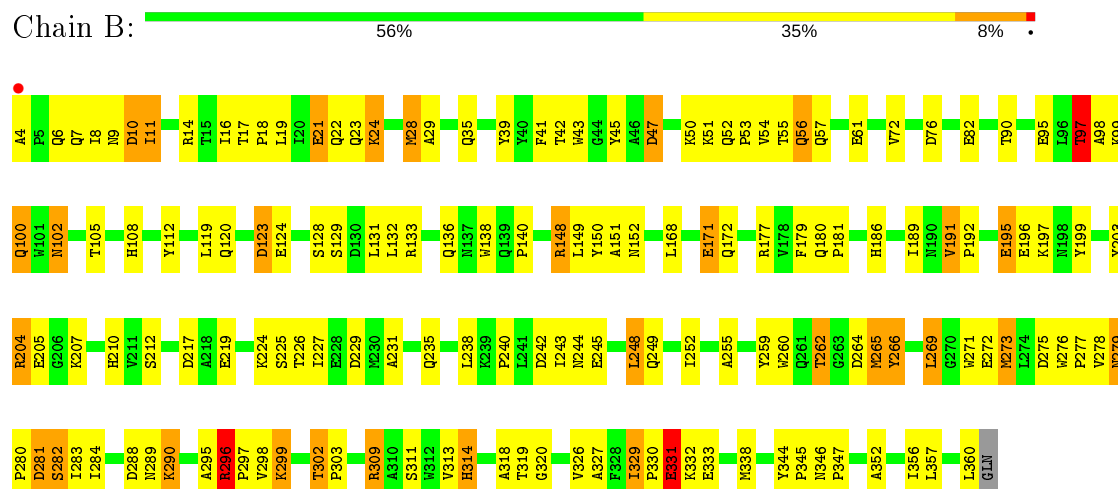
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: AMPC BETA-LACTAMASE



#### • Molecule 1: AMPC BETA-LACTAMASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.38Å 78.97Å 99.30Å 90.00° 116.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.56 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.00-2.30) 80.6 (25.56-1.97)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	136.72 (at 1.96Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.159 , (Not available) 0.149 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 109.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.18	12/2870 (0.4%)	1.47	27/3921 (0.7%)
1	B	1.16	12/2870 (0.4%)	1.52	30/3921 (0.8%)
All	All	1.17	24/5740 (0.4%)	1.50	57/7842 (0.7%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	GLU	CD-OE1	8.06	1.34	1.25
1	B	171	GLU	CD-OE2	7.91	1.34	1.25
1	B	331	GLU	CD-OE1	7.61	1.34	1.25
1	A	331	GLU	CD-OE1	7.32	1.33	1.25
1	B	205	GLU	CD-OE1	7.28	1.33	1.25
1	B	196	GLU	CD-OE2	7.10	1.33	1.25
1	B	95	GLU	CD-OE2	6.65	1.32	1.25
1	A	196	GLU	CD-OE2	6.64	1.32	1.25
1	A	171	GLU	CD-OE2	6.25	1.32	1.25
1	B	333	GLU	CD-OE1	6.24	1.32	1.25
1	A	333	GLU	CD-OE1	6.23	1.32	1.25
1	B	245	GLU	CD-OE2	6.15	1.32	1.25
1	A	205	GLU	CD-OE1	6.13	1.32	1.25
1	A	245	GLU	CD-OE2	6.10	1.32	1.25
1	A	228	GLU	CD-OE2	5.90	1.32	1.25
1	A	21	GLU	CD-OE1	5.88	1.32	1.25
1	A	95	GLU	CD-OE2	5.84	1.32	1.25
1	A	272	GLU	CD-OE1	5.78	1.32	1.25
1	A	219	GLU	CD-OE2	5.67	1.31	1.25
1	B	61	GLU	CD-OE2	5.43	1.31	1.25
1	B	124	GLU	CD-OE2	-5.40	1.19	1.25
1	A	272	GLU	CD-OE2	-5.36	1.19	1.25
1	B	82	GLU	CD-OE1	-5.14	1.20	1.25
1	B	195	GLU	CD-OE2	-5.10	1.20	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	199	TYR	CB-CG-CD2	-9.50	115.30	121.00
1	B	264	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	B	76	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	B	199	TYR	CB-CG-CD1	8.58	126.15	121.00
1	B	319	THR	CA-CB-CG2	-8.55	100.43	112.40
1	A	264	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	A	275	ASP	CB-CG-OD1	-8.30	110.83	118.30
1	B	217	ASP	CB-CG-OD1	8.17	125.65	118.30
1	A	177	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	133	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	177	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	258	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	A	242	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	56	GLN	CA-CB-CG	-7.08	97.83	113.40
1	A	217	ASP	CB-CG-OD1	7.07	124.67	118.30
1	B	296	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	296	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	148	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	281	ASP	CB-CG-OD1	-6.45	112.49	118.30
1	B	281	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	334	LEU	CB-CA-C	-6.38	98.07	110.20
1	B	224	LYS	N-CA-CB	6.34	122.01	110.60
1	B	123	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	A	242	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	29	ALA	N-CA-CB	6.27	118.88	110.10
1	A	47	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	288	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	97	THR	N-CA-CB	-6.09	98.73	110.30
1	A	130	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	87	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	76	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	10	ASP	CB-CG-OD1	-5.92	112.98	118.30
1	B	242	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	326	VAL	CG1-CB-CG2	-5.83	101.56	110.90
1	B	264	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	351	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	B	47	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	351	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	338	MET	CA-CB-CG	-5.70	103.61	113.30
1	A	76	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	72	VAL	CA-CB-CG1	-5.61	102.49	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	B	266	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	288	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	130	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	A	80	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	322	PHE	CB-CA-C	-5.26	99.88	110.40
1	A	349	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	242	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	28	MET	CG-SD-CE	-5.19	91.89	100.20
1	B	296	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	112	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	B	210	HIS	CA-CB-CG	-5.09	104.94	113.60
1	A	260	TRP	CB-CA-C	-5.05	100.30	110.40
1	B	203	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	B	275	ASP	CB-CG-OD1	-5.04	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2790	0	2769	106	0
1	B	2790	0	2769	109	0
2	A	10	0	8	1	0
2	B	10	0	8	3	0
3	A	57	0	0	2	0
3	B	50	0	0	2	0
All	All	5707	0	5554	215	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HD11	1:B:360:LEU:HD21	1.39	1.03
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.34	0.92
1:B:120:GLN:HE22	1:B:152:ASN:HD22	1.22	0.88
1:B:120:GLN:NE2	1:B:152:ASN:HD22	1.72	0.87
1:B:240:PRO:HA	1:B:243:ILE:HD12	1.57	0.86
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.59	0.83
1:B:11:ILE:CD1	1:B:360:LEU:HD21	2.10	0.81
1:A:240:PRO:HA	1:A:243:ILE:CD1	2.11	0.80
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.46	0.80
1:A:240:PRO:HA	1:A:243:ILE:HD12	1.65	0.79
1:A:169:SER:OG	1:A:172:GLN:HG3	1.82	0.78
1:B:238:LEU:HD23	1:B:330:PRO:HA	1.65	0.77
1:B:280:PRO:O	1:B:284:ILE:HG13	1.86	0.76
1:A:76:ASP:O	1:A:80:ARG:HG3	1.87	0.74
1:B:105:THR:H	1:B:108:HIS:CD2	2.07	0.73
1:B:105:THR:H	1:B:108:HIS:HD2	1.36	0.72
1:B:262:THR:HG23	1:B:297:PRO:O	1.90	0.72
1:A:64:SER:HB2	1:A:317:GLY:HA2	1.72	0.71
1:A:278:VAL:O	1:A:280:PRO:HD3	1.91	0.70
1:B:120:GLN:HE22	1:B:152:ASN:ND2	1.89	0.70
1:A:120:GLN:HE22	1:A:152:ASN:HD22	1.39	0.69
1:A:238:LEU:HD23	1:A:330:PRO:HA	1.74	0.68
1:B:279:ASN:OD1	1:B:282:SER:HB2	1.92	0.68
1:A:11:ILE:CD1	1:A:360:LEU:HD21	2.24	0.68
1:B:16:ILE:O	1:B:19:LEU:HB3	1.93	0.67
1:B:295:ALA:O	1:B:296:ARG:HD3	1.94	0.67
1:A:11:ILE:HD12	1:A:360:LEU:HD21	1.75	0.67
1:B:97:THR:HG22	1:B:136:GLN:HE22	1.59	0.67
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.77	0.67
1:A:105:THR:H	1:A:108:HIS:CD2	2.13	0.66
1:A:280:PRO:O	1:A:284:ILE:HG13	1.96	0.66
1:B:271:TRP:O	1:B:273:MET:HE3	1.96	0.66
1:A:171:GLU:O	1:A:175:GLN:HG3	1.96	0.65
1:A:172:GLN:O	1:A:176:THR:HG23	1.96	0.65
1:A:344:TYR:HB2	1:A:345:PRO:HD2	1.77	0.65
1:A:265:MET:HG2	1:A:266:TYR:N	2.12	0.65
1:B:279:ASN:HD21	1:B:281:ASP:HB2	1.61	0.64
1:A:120:GLN:NE2	1:A:152:ASN:HD22	1.95	0.64
1:B:231:ALA:O	1:B:235:GLN:HG3	1.98	0.63
1:B:7:GLN:O	1:B:11:ILE:HG13	1.98	0.63
1:A:47:ASP:OD2	1:A:50:LYS:NZ	2.29	0.63
1:B:344:TYR:HB2	1:B:345:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:NH1	1:B:331:GLU:HA	2.14	0.63
1:A:98:ALA:HB1	1:A:100:GLN:OE1	1.99	0.63
1:B:180:GLN:N	1:B:181:PRO:HD2	2.13	0.63
1:B:346:ASN:HB2	1:B:347:PRO:HD3	1.81	0.62
1:A:279:ASN:O	1:A:282:SER:HB2	2.01	0.61
1:A:295:ALA:O	1:A:296:ARG:HD3	2.00	0.61
1:B:265:MET:HE1	1:B:272:GLU:HG2	1.83	0.61
1:A:56:GLN:NE2	1:A:228:GLU:OE2	2.36	0.59
1:B:255:ALA:HA	1:B:269:LEU:HB2	1.85	0.59
1:B:240:PRO:HA	1:B:243:ILE:CD1	2.30	0.59
1:A:120:GLN:HE22	1:A:152:ASN:ND2	2.00	0.59
1:B:19:LEU:HD12	1:B:19:LEU:O	2.02	0.59
1:A:93:TRP:CZ2	1:A:132:LEU:HB2	2.39	0.58
1:A:240:PRO:CA	1:A:243:ILE:HD12	2.33	0.58
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.39	0.58
1:A:185:ASN:HB2	3:A:416:HOH:O	2.03	0.58
1:A:262:THR:HG23	1:A:297:PRO:O	2.04	0.58
1:B:288:ASP:OD1	1:B:290:LYS:HG2	2.04	0.57
1:A:217:ASP:O	1:A:218:ALA:C	2.39	0.57
1:B:120:GLN:NE2	1:B:152:ASN:ND2	2.47	0.57
1:B:11:ILE:CD1	1:B:360:LEU:HD11	2.35	0.57
1:A:17:THR:HB	1:A:18:PRO:HD3	1.87	0.57
1:A:296:ARG:HG3	1:A:296:ARG:NH1	2.11	0.56
1:B:204:ARG:HB2	1:B:320:GLY:O	2.06	0.55
1:B:4:ALA:HB2	1:B:39:TYR:CD2	2.41	0.55
1:B:240:PRO:O	1:B:249:GLN:HG3	2.07	0.55
1:B:90:THR:HG23	3:B:378:HOH:O	2.07	0.54
1:A:224:LYS:N	1:A:224:LYS:HD2	2.22	0.54
1:A:265:MET:HE3	1:A:272:GLU:CG	2.37	0.54
1:B:52:GLN:CD	1:B:53:PRO:HD2	2.28	0.54
1:A:105:THR:H	1:A:108:HIS:HD2	1.53	0.54
1:A:280:PRO:HG3	1:A:354:TRP:CH2	2.42	0.54
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.43	0.54
1:B:260:TRP:O	1:B:266:TYR:HA	2.07	0.54
1:A:104:ILE:HA	1:A:108:HIS:HD2	1.73	0.54
1:B:192:PRO:HD2	1:B:195:GLU:HB2	1.89	0.54
1:B:186:HIS:N	1:B:229:ASP:OD2	2.39	0.53
1:B:313:VAL:O	1:B:327:ALA:HA	2.07	0.53
1:B:265:MET:CE	1:B:272:GLU:HG2	2.38	0.53
1:B:318:ALA:N	2:B:362:APB:H2	2.23	0.53
1:B:11:ILE:HD12	1:B:360:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:HD13	1:B:252:ILE:HD12	1.90	0.52
1:B:119:LEU:HA	1:B:151:ALA:HA	1.92	0.52
1:B:240:PRO:CA	1:B:243:ILE:HD12	2.34	0.52
1:A:6:GLN:O	1:A:7:GLN:C	2.47	0.52
1:B:98:ALA:HB1	1:B:100:GLN:OE1	2.10	0.52
1:B:45:TYR:HA	1:B:53:PRO:HA	1.90	0.52
1:A:240:PRO:O	1:A:243:ILE:HD12	2.09	0.52
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.45	0.52
1:B:148:ARG:HB2	1:B:298:VAL:HG11	1.91	0.51
1:B:42:THR:HB	1:B:54:VAL:HG12	1.92	0.51
1:A:193:PRO:HA	1:A:196:GLU:HG3	1.93	0.51
1:A:353:ALA:O	1:A:357:LEU:HB2	2.11	0.51
1:B:4:ALA:HB2	1:B:39:TYR:HD2	1.74	0.50
1:A:125:VAL:HG13	1:A:130:ASP:HB3	1.92	0.50
1:A:217:ASP:OD1	1:A:218:ALA:N	2.43	0.50
1:B:219:GLU:N	1:B:219:GLU:OE1	2.36	0.50
1:A:271:TRP:O	1:A:273:MET:HE1	2.12	0.50
1:A:296:ARG:HH11	1:A:296:ARG:CG	2.14	0.50
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.10	0.50
1:A:271:TRP:HB2	1:A:273:MET:HE2	1.94	0.49
1:B:41:PHE:HB2	1:B:43:TRP:CZ3	2.48	0.49
1:A:175:GLN:HB3	1:A:180:GLN:NE2	2.27	0.49
1:B:243:ILE:CD1	1:B:252:ILE:HD12	2.43	0.49
1:B:23:GLN:O	1:B:24:LYS:HB2	2.12	0.49
1:B:352:ALA:O	1:B:356:ILE:HG13	2.12	0.48
1:A:264:ASP:OD1	1:A:264:ASP:N	2.36	0.48
1:B:171:GLU:HG3	1:B:189:ILE:HB	1.95	0.48
1:A:243:ILE:HD13	1:A:252:ILE:HD12	1.95	0.48
1:A:318:ALA:N	2:A:362:APB:H2	2.28	0.48
1:B:47:ASP:OD2	1:B:50:LYS:NZ	2.36	0.48
1:A:279:ASN:ND2	1:A:282:SER:H	2.12	0.48
1:B:259:TYR:CE1	1:B:269:LEU:HD13	2.48	0.48
1:B:296:ARG:NH1	1:B:296:ARG:HG3	2.21	0.48
1:B:344:TYR:HB2	1:B:345:PRO:CD	2.43	0.48
1:B:55:THR:C	1:B:57:GLN:H	2.15	0.48
1:A:265:MET:CE	1:A:272:GLU:HG2	2.44	0.48
1:B:41:PHE:HB3	1:B:43:TRP:CH2	2.48	0.48
1:A:271:TRP:C	1:A:273:MET:HE1	2.34	0.47
1:B:311:SER:O	1:B:329:ILE:HG23	2.14	0.47
1:A:10:ASP:O	1:A:14:ARG:HB2	2.14	0.47
1:A:179:PHE:CD1	1:A:179:PHE:N	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:PRO:C	1:A:243:ILE:HD12	2.35	0.47
1:B:238:LEU:CD2	1:B:330:PRO:HA	2.40	0.47
1:A:80:ARG:HD3	1:A:80:ARG:HH11	1.52	0.47
1:B:100:GLN:OE1	1:B:100:GLN:N	2.29	0.47
1:B:17:THR:N	1:B:18:PRO:HD2	2.30	0.47
1:A:197:LYS:HD2	3:A:395:HOH:O	2.14	0.47
1:A:119:LEU:HA	1:A:151:ALA:HA	1.96	0.47
1:A:118:PRO:O	1:A:151:ALA:HB1	2.15	0.46
1:B:346:ASN:N	1:B:347:PRO:CD	2.77	0.46
1:A:85:LEU:HB3	1:A:107:LEU:HB2	1.96	0.46
1:A:346:ASN:N	1:A:347:PRO:CD	2.79	0.46
1:A:278:VAL:HG22	1:A:279:ASN:N	2.30	0.46
1:B:302:THR:HA	1:B:303:PRO:HA	1.75	0.46
1:A:344:TYR:HB2	1:A:345:PRO:CD	2.44	0.46
1:A:329:ILE:O	1:A:330:PRO:C	2.50	0.46
1:B:10:ASP:HB3	1:B:14:ARG:NH1	2.31	0.45
1:B:4:ALA:CB	1:B:39:TYR:CD2	2.99	0.45
1:B:41:PHE:CB	1:B:43:TRP:CH2	3.00	0.45
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.61	0.45
1:A:171:GLU:HG3	1:A:189:ILE:HD12	1.99	0.45
1:B:289:ASN:HA	1:B:289:ASN:HD22	1.42	0.45
1:B:271:TRP:HB2	1:B:273:MET:HE1	1.99	0.45
1:A:309:ARG:NH1	1:A:331:GLU:HA	2.32	0.45
1:B:8:ILE:O	1:B:9:ASN:C	2.54	0.45
1:A:17:THR:N	1:A:18:PRO:HD2	2.32	0.44
1:B:191:VAL:HA	1:B:192:PRO:HD3	1.86	0.44
1:B:29:ALA:C	1:B:227:ILE:HD13	2.38	0.44
1:B:56:GLN:HG3	3:B:366:HOH:O	2.17	0.44
1:B:225:SER:OG	1:B:226:THR:N	2.49	0.44
1:A:182:LEU:O	1:A:183:LYS:HB2	2.17	0.44
1:B:309:ARG:O	1:B:331:GLU:HB3	2.17	0.44
1:A:110:ALA:HB2	1:A:158:PHE:CD1	2.53	0.44
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.31	0.44
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.87	0.44
1:B:39:TYR:N	1:B:39:TYR:CD1	2.86	0.43
1:A:100:GLN:C	1:A:102:ASN:H	2.22	0.43
1:A:204:ARG:HB2	1:A:320:GLY:O	2.18	0.43
1:B:138:TRP:CH2	1:B:140:PRO:HB3	2.53	0.43
1:B:41:PHE:CD1	1:B:41:PHE:N	2.86	0.43
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.72	0.43
1:B:19:LEU:HD12	1:B:19:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:CB	1:A:273:MET:CE	2.97	0.43
1:A:313:VAL:O	1:A:327:ALA:HA	2.19	0.43
1:B:150:TYR:CE2	2:B:362:APB:H6	2.54	0.43
1:B:318:ALA:HB2	2:B:362:APB:HN11	1.83	0.43
1:B:52:GLN:NE2	1:B:52:GLN:HA	2.33	0.43
1:B:17:THR:HB	1:B:18:PRO:HD3	2.01	0.43
1:B:299:LYS:HB2	1:B:299:LYS:HE3	1.71	0.43
1:B:278:VAL:HG22	1:B:279:ASN:N	2.34	0.42
1:B:279:ASN:ND2	1:B:281:ASP:HB2	2.31	0.42
1:B:6:GLN:HA	1:B:9:ASN:HB2	2.00	0.42
1:B:52:GLN:OE1	1:B:53:PRO:HD2	2.18	0.42
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.76	0.42
1:A:41:PHE:HB2	1:A:43:TRP:CZ3	2.53	0.42
1:A:204:ARG:HH11	1:A:204:ARG:CG	2.33	0.42
1:A:278:VAL:CG2	1:A:279:ASN:N	2.82	0.42
1:B:123:ASP:N	1:B:123:ASP:OD1	2.52	0.42
1:A:180:GLN:N	1:A:181:PRO:CD	2.81	0.42
1:A:265:MET:HE3	1:A:272:GLU:HG2	2.01	0.42
1:B:100:GLN:CD	1:B:100:GLN:H	2.19	0.42
1:B:112:TYR:HB3	1:B:149:LEU:O	2.20	0.42
1:B:265:MET:HG3	1:B:266:TYR:N	2.34	0.42
1:B:271:TRP:HB2	1:B:273:MET:CE	2.49	0.42
1:B:41:PHE:CB	1:B:43:TRP:CZ3	3.02	0.42
1:B:240:PRO:O	1:B:243:ILE:HD12	2.19	0.42
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.77	0.42
1:A:149:LEU:O	1:A:150:TYR:C	2.58	0.42
1:B:171:GLU:HG3	1:B:189:ILE:HD12	2.01	0.42
1:B:271:TRP:CB	1:B:273:MET:CE	2.98	0.42
1:A:33:ILE:O	1:A:334:LEU:HA	2.20	0.41
1:A:23:GLN:O	1:A:24:LYS:HB2	2.21	0.41
1:A:7:GLN:O	1:A:11:ILE:HG13	2.20	0.41
1:A:94:PRO:HD2	1:A:95:GLU:OE2	2.21	0.41
1:A:240:PRO:O	1:A:249:GLN:HG3	2.19	0.41
1:A:265:MET:HE3	1:A:272:GLU:CD	2.41	0.41
1:A:258:ARG:HH11	1:A:258:ARG:HD3	1.66	0.41
1:A:267:GLN:HG3	1:A:268:GLY:O	2.21	0.41
1:A:314:HIS:HB2	1:A:326:VAL:O	2.20	0.41
1:A:93:TRP:O	1:A:96:LEU:HB2	2.19	0.41
1:A:16:ILE:HG22	1:A:20:ILE:CD1	2.51	0.41
1:B:179:PHE:CD1	1:B:179:PHE:N	2.84	0.41
1:A:271:TRP:HB3	1:A:273:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:MET:CE	1:A:272:GLU:HB3	2.51	0.41
1:A:271:TRP:CB	1:A:273:MET:HE2	2.50	0.41
1:A:346:ASN:O	1:A:350:VAL:HG23	2.21	0.40
1:B:314:HIS:HB2	1:B:326:VAL:O	2.21	0.40
1:A:168:LEU:HD22	1:A:172:GLN:NE2	2.37	0.40
1:A:289:ASN:HA	1:A:289:ASN:HD22	1.27	0.40
1:A:30:VAL:HG12	1:A:31:ALA:N	2.36	0.40
1:B:28:MET:HG3	1:B:29:ALA:N	2.37	0.40
1:B:56:GLN:HB2	1:B:57:GLN:NE2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	355/358 (99%)	340 (96%)	14 (4%)	1 (0%)	41	50
1	B	355/358 (99%)	330 (93%)	24 (7%)	1 (0%)	41	50
All	All	710/716 (99%)	670 (94%)	38 (5%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ASN
1	A	102	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/292 (100%)	253 (87%)	38 (13%)	4	4
1	B	291/292 (100%)	252 (87%)	39 (13%)	4	4
All	All	582/584 (100%)	505 (87%)	77 (13%)	4	4

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	21	GLU
1	A	22	GLN
1	A	24	LYS
1	A	35	GLN
1	A	51	LYS
1	A	97	THR
1	A	99	LYS
1	A	100	GLN
1	A	102	ASN
1	A	123	ASP
1	A	124	GLU
1	A	129	SER
1	A	132	LEU
1	A	164	LYS
1	A	168	LEU
1	A	172	GLN
1	A	191	VAL
1	A	197	LYS
1	A	204	ARG
1	A	207	LYS
1	A	241	LEU
1	A	248	LEU
1	A	262	THR
1	A	265	MET
1	A	269	LEU
1	A	273	MET
1	A	279	ASN
1	A	282	SER
1	A	283	ILE
1	A	296	ARG
1	A	299	LYS
1	A	302	THR

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Mol	Chain	Res	Type
1	A	309	ARG
1	A	314	HIS
1	A	331	GLU
1	A	332	LYS
1	A	357	LEU
1	B	11	ILE
1	B	21	GLU
1	B	22	GLN
1	B	24	LYS
1	B	35	GLN
1	B	51	LYS
1	B	97	THR
1	B	99	LYS
1	B	100	GLN
1	B	102	ASN
1	B	128	SER
1	B	129	SER
1	B	132	LEU
1	B	168	LEU
1	B	172	GLN
1	B	191	VAL
1	B	197	LYS
1	B	204	ARG
1	B	207	LYS
1	B	212	SER
1	B	244	ASN
1	B	248	LEU
1	B	262	THR
1	B	265	MET
1	B	269	LEU
1	B	273	MET
1	B	279	ASN
1	B	282	SER
1	B	283	ILE
1	B	290	LYS
1	B	296	ARG
1	B	299	LYS
1	B	302	THR
1	B	309	ARG
1	B	314	HIS
1	B	329	ILE
1	B	331	GLU

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Mol	Chain	Res	Type
1	B	332	LYS
1	B	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	23	GLN
1	A	52	GLN
1	A	108	HIS
1	A	120	GLN
1	A	147	GLN
1	A	172	GLN
1	A	180	GLN
1	A	279	ASN
1	A	289	ASN
1	B	23	GLN
1	B	52	GLN
1	B	56	GLN
1	B	57	GLN
1	B	108	HIS
1	B	120	GLN
1	B	137	ASN
1	B	172	GLN
1	B	175	GLN
1	B	180	GLN
1	B	289	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	APB	A	362	1	10,10,10	7.42	3 (30%)	13,13,13	2.27	5 (38%)
2	APB	B	362	1	10,10,10	7.65	3 (30%)	13,13,13	2.09	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APB	A	362	1	-	2/4/4/4	0/1/1/1
2	APB	B	362	1	-	2/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	362	APB	B-O2	18.26	1.67	1.36
2	A	362	APB	B-O2	18.10	1.67	1.36
2	B	362	APB	B-O1	14.06	1.60	1.36
2	A	362	APB	B-O1	14.03	1.60	1.36
2	B	362	APB	B-C1	7.25	1.71	1.57
2	A	362	APB	B-C1	5.08	1.67	1.57

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	APB	O1-B-C1	-5.47	103.63	119.95
2	A	362	APB	O2-B-C1	-4.50	106.51	119.95
2	A	362	APB	O1-B-C1	-4.20	107.41	119.95
2	B	362	APB	O2-B-C1	-3.37	109.88	119.95
2	A	362	APB	C6-C1-C2	2.91	120.51	117.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	362	APB	O2-B-O1	-2.75	110.40	119.67
2	A	362	APB	C5-C6-C1	-2.75	118.85	121.57
2	B	362	APB	O2-B-O1	-2.54	111.12	119.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	362	APB	O2-B-C1-C2
2	A	362	APB	O2-B-C1-C6
2	B	362	APB	O2-B-C1-C2
2	B	362	APB	O2-B-C1-C6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	362	APB	1	0
2	B	362	APB	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	357/358 (99%)	-1.09	0 <span>100</span> <span>100</span>	4, 16, 55, 77	4 (1%)
1	B	357/358 (99%)	-1.03	1 (0%) <span>94</span> <span>96</span>	4, 17, 56, 79	4 (1%)
All	All	714/716 (99%)	-1.06	1 (0%) <span>95</span> <span>97</span>	4, 17, 56, 79	8 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	ALA	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	APB	B	362	10/10	0.78	0.25	24,69,100,100	0
2	APB	A	362	10/10	0.81	0.23	23,68,100,100	0

## 6.5 Other polymers

There are no such residues in this entry.